

Claims

I claim:

1           1. A method of measuring the molecular mass of a compound Y of unknown  
2 molecular mass by mass spectrometry, comprising  
3           providing a sample of compound Y,  
4           providing samples of at least two different compounds each of Formula (I), R-X in  
5 which R is a trityl group and X is cleavable to form a charged species for mass spectrometry,  
6           and recording the molecular mass of compound Y and the at least two compounds  
7 of Formula (I) in a mass spectrometer.

1           2. The method, according to claim 1, in which R is  $R^1R^2R^3$  C- wherein  $R^1$ ,  $R^2$  and  
2  $R^3$  are the same or different and each is a monocyclic or fused ring aromatic group that is  
3 substituted or unsubstituted.

1           3. The method, according to claim 2, in which at least one of  $R^1$ ,  $R^2$  and  $R^3$  carries  
2 a substituent selected from the group consisting of substituted or unsubstituted  $C_1$ - $C_{20}$  alkoxy  
3 and hydrocarbyl.

1           4. The method, according to claim 3, in which the alkoxy or hydrocarbyl is  
2 substituted by a substituent selected from the group consisting of carboxylic acid, sulphonic  
3 acid, nitro, cyano, hydroxyl, thiol, primary, secondary or tertiary amino, primary or secondary  
4 amido, anhydride, carbonyl halide and active ester.

1           5. The method, according to any of claim 2, in which each of  $R^1$ ,  $R^2$  and  $R^3$  is aryl.

1           6. The method, according to claim 5, wherein said aryl is phenyl.

1           7. The method, according to claim 1, in which the trityl group R has at least two  
2 amide substituents.

1           8. The method, according to claim 7, wherein said trityl group R has at least four  
2 amide substituents.

1           9. The method, according claim 2, in which  $R^1$ ,  $R^2$  and  $R^3$  together carry at least two  
2 amide groups and/or at least two reactive groups for coupling.

1           10. The method, according to claim 9, wherein said groups are N-hydroxy  
2 succinimide ester groups.

1           11. The method, according to claim 1, in which X is halide or tosylate.

1           12. The method, according to claim 1, comprising providing at least five compounds  
2 of Formula (I) and recording their molecular masses in a mass spectrometer.

1           13. The method, according claim 1, in which the group X is photocleavable to form  
2 a charged species for mass spectrometry.

1           14. The method, according to claim 1, additionally comprising estimating the  
2 molecular mass of unknown compound Y as  $M_y$  and providing at least one compound of  
3 Formula (I) which has known molecular mass  $M_1$  below  $M_y$  and at least one different  
4 compound of Formula (I) which has molecular mass  $M_2$  above  $M_y$ .

1           15. The method, according to claim 14, wherein the difference between  $M_y$  and each  
2 of  $M_1$  and  $M_2$  is not more than  $\pm 50\%$ .

1           16. The method, according to claim 1, additionally comprising providing a sample  
2 of at least one further compound Z of unknown molecular mass and measuring the molecular  
3 mass of compound Z.

1           17. Use of a compound of Formula (I) R-X in which R is a trityl group and X is  
2 cleavable to form a charged species for mass spectrometry as a calibration compound for  
3 mass spectrometry.

1           18. A kit for the production of calibration compounds for mass spectrometry  
2 comprising:

3           (a) at least one base reactant of Formula (I) R-X where R is a trityl group and X is  
4 cleavable to form a charged species for mass spectrometry; and

5           (b) at least two different amine compounds which are of different molecular masses  
6 and which are each capable of reacting with the base reactant;

7           wherein the base reactant (a) is packaged separately from amine compounds (b).

1           19. The kit, according to claim 18, additionally comprising instructions to select at  
2 least two desired molecular masses  $M_1$  and  $M_2$  for the calibration compounds and to choose  
3 one or more amines for reaction with the base reactant so as to obtain compounds of the  
4 desired predetermined molecular masses  $M_1$  and  $M_2$ , and instructions to use the compounds  
5 in mass spectrometry.

1           20. A set of calibration compounds for mass spectrometry comprising at least two  
2 separately packaged mixtures (a) and (b), wherein

3           mixture (a) comprises at least two different compounds each of formula (I) R-X and  
4 having different molecular masses, and

5           mixture (b) comprises at least two further compounds of formula (I) R-X having  
6 different molecular masses and wherein R is a trityl group and X is cleavable to form a  
7 charged species for mass spectrometry.

1           21. The set, according to claim 20, in which the lowest molecular mass in mixture  
2 (a) is lower than the lowest molecular mass in mixture (b) and the highest molecular mass  
3 in mixture (a) is lower than the highest molecular mass in mixture (b).

1           22. The set, according to claim 20, in which each of mixtures (a) and (b) contains at  
2 least five different compounds of different molecular masses.

1           23. The set, according to claim 22, in which each of mixtures (a) and (b) contains at  
2 least 10 different compounds of different molecular masses.

1           24. The set, according to claim 20, comprising at least three separately packaged  
2 mixtures of compounds.

1           25. The set, according to claim 24, comprising at least five separately packaged  
2 mixtures of compounds.

1           26. A kit for the production of a set of calibration compounds comprising a first  
2 package comprising a base reactant of Formula (I) R-X, in which R is a trityl group and X  
3 is cleavable to form a charged species for mass spectrometry, and at least two separate  
4 second packages (a) and (b), each containing a mixture of at least two amine compounds  
5 which have different molecular masses and which are capable of reacting with the base  
6 reactant.

1           27. The kit, according to claim 26, in which the lowest molecular mass in mixture  
2 (a) is lower than the lowest molecular mass in mixture (b) and the highest molecular mass  
3 in mixture (a) is lower than the highest molecular mass in mixture (b).

1           28. The kit, according to claim 26, in which each of mixtures (a) and (b) contain at  
2           least five different amine compounds of different molecular masses.

1           29. The kit, according to claim 28, wherein each of mixtures (a) and (b) contain at  
2           least ten different amine compounds of molecular masses.

1           30. The kit, according to claim 26, comprising at least three mixtures of amine  
2           compounds.

1           31. The kit, according to claim 30, comprising at least five mixtures of amine  
2           compounds.

1           32. A method of measuring the molecular mass of a compound Y of unknown  
2           molecular mass comprising  
3           estimating the expected molecular mass of compound Y, selecting at least one  
4           calibration compound of Formula (I) R-X having molecular weight close to the expected  
5           molecular weight of the compound Y, in which R is a trityl group and X is cleavable to form  
6           a charged species for mass spectrometry  
7           and subjecting both compounds to mass spectrometry simultaneously.

1           33. The method, according to claim 32, in which the calibration compound R-X is  
2           provided by selecting a base reactant R-X and selecting an amine reactant of appropriate  
3           molecular mass and reacting the amine reactant and the base reactant.

1           34. A mixture of at least two compounds of Formula (I) R-X in which R is a trityl  
2           group and X is a group cleavable to give a charged species for analysis by mass spectrometry.

1           35. The mixture, according to claim 34, comprising at least five different compounds  
2           of Formula (I).

1           36. The mixture, according to claim 35, comprising at least ten different compounds  
2 of Formula (I).

1           37. A method of mass spectrometry comprising subjecting simultaneously to mass  
2 spectrometry at least two different compounds of Formula (I) R-X in which R is a trityl  
3 group and X is cleavable to give a charged species for analysis by mass spectrometry.